SELECTIVE EMITTERS USING PHOTONIC CRYSTALS FOR THERMOPHOTOVOLTAIC ENERGY CONVERSION

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ABSTRACT

Photonic crystals use a periodic modulation of the refractive index to alter the photonic density of states. The photonic density of states is an important parameter in many phenomena involving radiation-matter interactions – including thermal emission of radiation. Hence, a photonic crystal can be used to engineer the emissivity of an emitter for thermophotovoltaic generators to match the spectral response of the TPV cell. The use of photonic crystals in TPV is described. A three-dimensional photonic crystal in tungsten is realized that exhibits an exceptionally large photonic bandgap and attenuation factor. The photonic crystal is shown to have promise for radiant energy conversion applications like TPV energy conversion.

INTRODUCTION

Thermophotovoltaic (TPV) energy conversion converts the radiant energy of a high-temperature body ("emitter") directly into electricity using a photovoltaic cell. TPV has a number of attractive features, including: fuel versatility (nuclear, fossil, solar, etc.), quiet operation, low maintenance, low emissions, light weight, high power density, modularity, and cogeneration of heat and power. TPV could potentially be used for distributed power, automotive, military, and other applications wherever fuel cells, microturbines, or cogeneration are presently being considered if the TPV efficiencies could be raised to around 30%. While the concept is very old, TPV is experiencing renewed interest due to recent advances in low-bandgap photovoltaic cells.[1] Low-bandgap photovoltaic cells are required to work with emitters at manageable temperatures (1300 to 1800K).

The efficiency of a TPV system could be significantly improved if the spectrum of the emitter could be tailored to match the peak response of the photovoltaic cell. For example, photovoltaic cells have energy-conversion efficiencies over 50% if illuminated with monochromatic light near the bandgap.[2] Spectral control can be achieved by either controlling the spectrum of the emitted radiation ("selective emitter") or by using spectral filters to return unwanted radiation to the emitter. Achieving high efficiencies requires very high performance in terms of the spectral selectivity or reflectivity, bandwidth, and the angular distribution with either a selective emitter or a spectral filter.[3]

Recently, the control of spectral emissivity by physically structuring the emitter has been examined by several researchers.[4,5] This is a new and powerful approach to controlling emissivity that can use well-established materials and tools from the microelectronics and thin-film industries.

We recently described a new approach for selective emissivity through the use of photonic crystals for TPV energy conversion.[6] This paper will provide an update on use of photonic crystals in TPV. We first describe the properties of photonic crystals. Next, we present some preliminary results using photonic crystals constructed using tungsten. Finally, we present the prospects of this approach for significantly improving TPV energy conversion efficiency.

PHOTONIC CRYSTALS and THERMAL EMISSION

Photonic crystals are structured materials where the refractive index is modulated in one, two, or three dimensions.[7] The modulation of the refractive index alters the photonic density-of-states spectrum. Many properties involving the interaction of radiation and materials, such as spontaneous or thermal emission of radiation, were once thought of as intrinsic properties of the material. However, these properties are, in fact, a function of the photonic density of states through Fermi's Golden Rule (Eq. 1).[8,9]

$$p_{i\to f}(\omega_k) \propto \rho(\omega_k)\cdot\left|\left\langle i\left|\mu\bullet E_k(\omega_k)\right|f\right\rangle\right|^2 \quad \textbf{Eq. 1.}$$

This equation represents the probability of a radiative transition from an initial state *i* to a final state *f* for optical mode ω_k. The term in the brackets is the quantum mechanical matrix element associated with the radiative transition, which is the product of the electric dipole moment μ and electric field E_k for optical mode ω_k. The matrix element is multiplied by the number of optical

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modes at ω_k – i.e., the photonic density of states $\rho(\omega_k)$—to get the transition rate.

The modification of thermal radiation can also be described with classical mechanics through the definition of emissivity.

$$I(\lambda,T) = \varepsilon(\lambda)\cdot I_{BB}(\lambda,T)$$
$$I_{BB}(\lambda,T) = \frac{2\pi hc^2}{\lambda^5(e^{\frac{hc}{\lambda kT}}-1)} \qquad \textbf{Eq. 2}$$

Eq. 2 states that the thermal radiation from a graybody is equal to the emissivity $\varepsilon(\lambda)$ multiplied by the thermal radiation from a blackbody $I_{BB}(\lambda)$ (Planck's Law). For purely thermal emission, it can be shown that the emissivity is equal to absorptivity (Kirchoff's Law), which provides a convenient method for calculating and measuring emissivity.[10] The quantum and classical descriptions are, of course, fully equivalent.[9]

The significance of this discussion is that the radiation-material interaction is subject to engineering through physical structuring of the material(s) into a photonic crystal.[8] It is even possible to design structures where there are no photonic states for a specific frequency range; i.e., a *photonic bandgap*. Such structures are said to exhibit a *full* photonic bandgap if there are no photonic states in any direction and for any polarization. (The *bandgap* terminology is borrowed from semiconductor physics where crystal symmetry leads to a similar gap in the density of states for electrons.) As implied by Eq. 1 and 2, the radiative transition probability and the spectral emissivity are zero within a *full* photonic bandgap. Photonic crystals therefore provide the ultimate control of emissivity since these structures can achieve a true photonic bandgap.

The important parameters of a photonic crystal include the crystal symmetry and lattice constant, which determine the bandgap of the photonic crystal, and the refractive index contrast, which determines the magnitude and bandwidth of the photonic bandgap. Three-dimensional photonic crystals can exhibit a full photonic bandgap. One- and two-dimensional photonic crystals generally do not exhibit a *full* photonic bandgap; rather, they generally exhibit a photonic bandgap only for a narrow range of angles and/or for specific polarizations.

We have previously demonstrated the alteration of thermal emission by a three-dimensional photonic crystal.[11] We fabricated and measured the thermal emission of a three-dimensional photonic crystal in polycrystalline silicon. Silicon behaves optically like a dielectric in the infrared. The thermal emission was suppressed in the photonic bandgap and was enhanced in the photonic passband, which matched the expected alteration of the photonic density of states in the silicon photonic crystal. Hence, the issue is developing and demonstrating the potential of a photonic crystal for enhancing TPV energy conversion.

EXPERIMENT

Practical TPV energy conversion systems require high emitter temperatures, e.g., around 1800K, to obtain high efficiencies and power densities. The high temperatures require refractory materials for the emitter. Tungsten is widely used in such refractory applications as incandescent light bulbs because the material is easily handled and can handle the high temperatures. Metals also offer the advantage of a very large refractive index contrast that enhances the effects of photonic structures. In particular, a large photonic bandgap is needed to suppress the long-wavelength infrared emission of a blackbody. Finally, tungsten is advantageous since it can be easily deposited and patterned using commonly available tools from the microelectronics industry.

We developed a process for producing three-dimensional tungsten photonic crystals using the basic process used to fabricate our three-dimensional polysilicon photonic crystals. The photonic crystal consists of a stack of layers with rods (Fig. 1). Each layer of rods is produced using common processes from the microelectronics industry -- oxide deposition, patterning to open a trench, polysilicon deposition in the trench, and chemical-mechanical polishing to planarize the surface. Layers of rods are sequentially fabricated and the oxide is removed at the end. The result is a face-centered cubic crystal.[12] The tungsten crystal is obtained by first fabricating a photonic crystal in polysilicon in a silicon dioxide matrix with the aforementioned fabrication sequence. The polysilicon is then removed with a chemical etch, which leaves a silicon-dioxide mold of the photonic crystal. Tungsten is deposited into this mold with chemical vapor deposition, and then the silicon dioxide mold is removed with a chemical etch.[13]

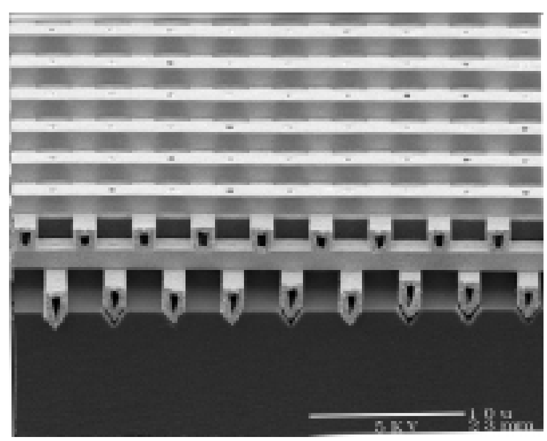

Figure 1. SEM photomicrograph of cross section of a 4-layer 3-dimensional tungsten photonic crystal. The photonic crystal has a lattice spacing of 4.2 μm and a diamond crystal symmetry. The tungsten rods are hollow due to poor step coverage of the tungsten CVD step.

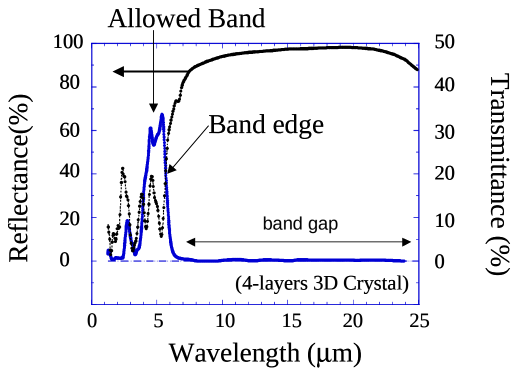

Figure 2. Spectral reflectance and transmittance of 4-layer 3-dimensional tungsten photonic crystal.

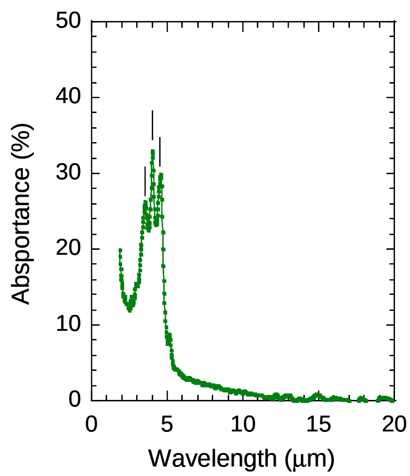

Figure 3. Spectral absorptance of 4-layer 3-dimensional tungsten photonic crystal.

The photonic crystals were characterized via reflectance, transmittance, and absorptance measurements using a Fourier-transform infrared measurement system (FTIR) from 1.5 to 25 μm (Fig 2 and 3). The metallic photonic crystal exhibited an enormous bandgap (around 8 to over 20 μm) and attenuation factor (30 dB per unit cell at 12 μm), as well as a transmittance and absorptance band near the edge of the photonic bandgap. The extremely large photonic bandgap and attenuation factor are due to the very large refractive index contrast using a metallic photonic crystal, while the absorption band is due to the unusual electromagnetic behavior associated with metallic photonic crystals. The fabrication, characterization, and, in particular, the unusual electromagnetic modes in metallic photonic crystals are described elsewhere.[13] We have also directly measured the emission of a tungsten photonic crystal that was heated electrically, and confirmed that the emission spectra matched the absorption spectra as expected from Eq. 2.[14]

RESULTS AND TPV MODEL

The present tungsten photonic crystal has a cutoff wavelength of around 8 μm. As is well known in photonic crystal physics, the cutoff wavelength can be moved to shorter wavelengths by using a smaller lattice constant for the photonic crystal. In order to compare the performance of a tungsten photonic crystal designed for TPV applications with other selective emitter approaches, we projected the spectral emissivity of a tungsten photonic crystal where the cutoff wavelength is moved to around 1.7 μm – which is the appropriate cutoff wavelength to use with a GaSb photovoltaic cell (E_g of 0.72 eV). This was achieved by: (1) equating the absorptivity with emissivity (Fig. 3), and (2) dividing the wavelength scale by 3.4. This scaling corresponds to a tungsten photonic crystal with a lattice constant of 1.2 μm, which is compatible with current fabrication technology. This scaling procedure was adopted since the dispersion relation in photonic crystals scales as the wavelength divided by the lattice constant.

We constructed a simple one-dimensional model of TPV energy conversion (Fig. 4). The purpose of the model is to compare the potential performance of a more optimal tungsten photonic crystal with other selective-emitter approaches that have been described in the literature. This model therefore does not include a model of the combustion process nor try to provide a realistic estimate of total system conversion efficiency. Rather, the model provides performance trends as a function of different spectral properties in the TPV system.

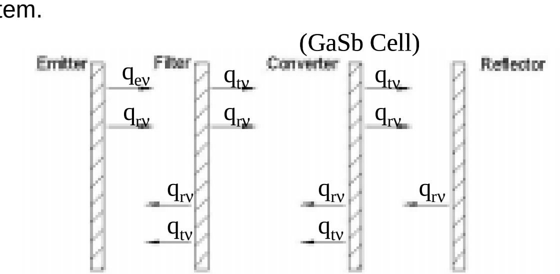

Figure 4. An illustration of radiative fluxes in a simple one-dimensional model of TPV energy conversion that includes only spectral effects.

The model for the GaSb photovoltaic cell and the TPV system is similar to the model described by Zenker *et al.*[2] We estimated the TPV efficiency (photovoltaic cell output divided by net radiant flux) with our scaled tungsten photonic crystal, with a microstructured tungsten emitter[3], with an erbia/yttria selective emitter, and with an ideal blackbody.

Our TPV system calculations found a much higher projected radiation-to-electricity conversion efficiency for the photonic crystal compared to the other selective-emitter approaches (Table 1). Note that the higher conversion efficiency was achieved at the expense of a reduced power density, which is an issue with any selective emitter and could potentially affect the economics of the TPV system.

CONCLUSION

Photonic crystals offer a completely new and powerful method for modifying the spectral emissivity of thermal emitters. Photonic crystals provide the ultimate control of emissivity since they can achieve a true photonic bandgap where there is a complete absence of photonic states. Spectrally selective emitters based on photonic crystals could be used to substantially enhance the efficiency of thermophotovoltaic energy converters, incandescent lamps, or any other application using high-temperature radiators.

Table 1. Results of TPV calculations using various emitters. Model used an 1800K radiator and GaSb photovoltaic cell.

Emitter	Radiant flux (W/cm^2)	Electric power (W/cm^2)	Eff. (%)
Blackbody	56.9	7.2	12.6
Photonic crystal	14.2	3.8	26.9
Microstructured W	19.6	4.4	22.4
Erbia/yttria	16.6	2.6	15.5

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